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Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 9.93

Global applicability domain: Inside

Local applicability domain index: 4.79e-01

Confidence level: 6.00e-01

Nearest Neighbors from the Training Set

Image not found
O,O-Diethyl dithiophosphate
Measured: 5.01
Predicted: 5.43

Image not found
Disulfoton
Measured: 219
Predicted: 151

Image not found
Isophorone
Measured: 2.00
Predicted: 3.19

Image not found
Menthol
Measured: 10.8
Predicted: 23.5

Image not found
(1R,2S,5R)-(-)-Menthol
Measured: 10.8
Predicted: 23.5

Image not found
Thiram
Measured: 3.39
Predicted: 3.91